WHAT IS CLAIMED IS:

1. A process for high throughput screening of binding of ligands to macromolecules using high resolution powder diffraction data comprising:

producing a first sample slurry of a selected polycrystalline macromolecule material and a solvent;

producing a second sample slurry of a selected polycrystalline macromolecule material, one or more ligands and said solvent;

obtaining a high resolution powder diffraction pattern on each of said first sample slurry and said second sample slurry; and,

comparing the high resolution powder diffraction pattern of said first sample slurry and the high resolution powder diffraction pattern of said second sample slurry whereby a difference in the high resolution powder diffraction patterns of said first sample slurry and said second sample slurry provides a positive indication for the formation of a complex between said selected polycrystalline macromolecule material and at least one of said one or more ligands.

2. The process of claim 1 wherein said macromolecule is a protein.

3. A process of high throughput screening of binding of ligands to macromolecules using high resolution powder diffraction data comprising:

producing a sample slurry mixture including a selected polycrystalline macromolecule material, a solvent, and a mixture of N ligands;

obtaining a high resolution powder diffraction pattern of said sample slurry mixture;

comparing the high resolution powder diffraction pattern of said sample slurry mixture with a reference of a high resolution powder diffraction pattern of said selected polycrystalline macromolecule material in the absence of any ligands whereby a difference in the high resolution powder diffraction patterns of said sample slurry mixture and said selected polycrystalline macromolecule material in the absence of any ligands provides a positive indication for the formation of a complex between said selected polycrystalline macromolecule material and at least one of said mixture of N ligands;

dividing said mixture of N ligands into at least two sample slurry groups by forming at least a first sample slurry including said selected polycrystalline macromolecule material, said solvent, and a mixture of selected ligands from among the N ligands, and forming at least a second sample slurry including said selected polycrystalline macromolecule material, said solvent, and a mixture of selected ligands not in said first sample slurry, wherein all of said N ligands are present in at least one of said sample slurry groups;

repeating steps of obtaining high resolution powder diffraction patterns, and steps of comparing said high resolution powder diffraction patterns whereby a difference in high resolution powder diffraction patterns between a said sample slurry and said selected polycrystalline macromolecule material in the absence of any ligands provides a positive indication for the formation of a complex between said selected polycrystalline macromolecule material and at least one ligand within a said sample slurry; and,

repeating steps of dividing said mixture of selected ligands for any sample slurry exhibiting a positive indication for the formation of a complex between said selected polycrystalline macromolecule material and at least one ligand within said sample slurry into at least two additional sample slurry groups, steps of obtaining high resolution powder diffraction patterns, and steps of comparing said high resolution powder diffraction patterns until all ligands within said mixture of N ligands that show binding have been identified.

4. The process of claim 3 wherein said macromolecule is a protein.

5. The process of claim 3 wherein where N is equal to 2^n and n is a positive integer.